Applying Leadership Computing to Supernova & Cosmology Simulations

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Argonne mechanical group: Vic Guarino, Tom Kasprzyk, Frank Skrzecz, Allen Zhao

Additional contributors: Eve Kovacs (Argonne), John Cunningham, Tara Hufford (Loyola Chicago), Ian Crane (U. Illinois)

Santa Fe Cosmology Workshop
St. John's College
Santa Fe, NM   July 22, 2010

Topics to Discuss

- Dark Energy Survey Supernovae
- Introduction to the Argonne Leadership Computing Facility
- Pursuing answers via high performance computing simulations
- Summary & conclusions

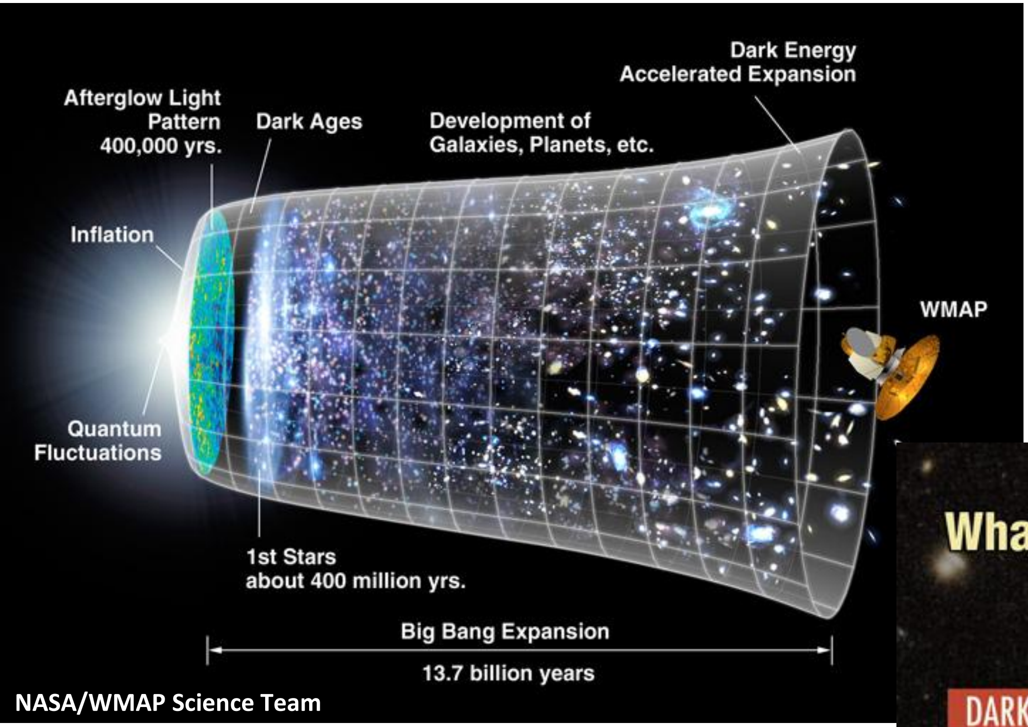
Argonne NATIONAL LABORATORY

Office of Science
U.S. Department of Energy

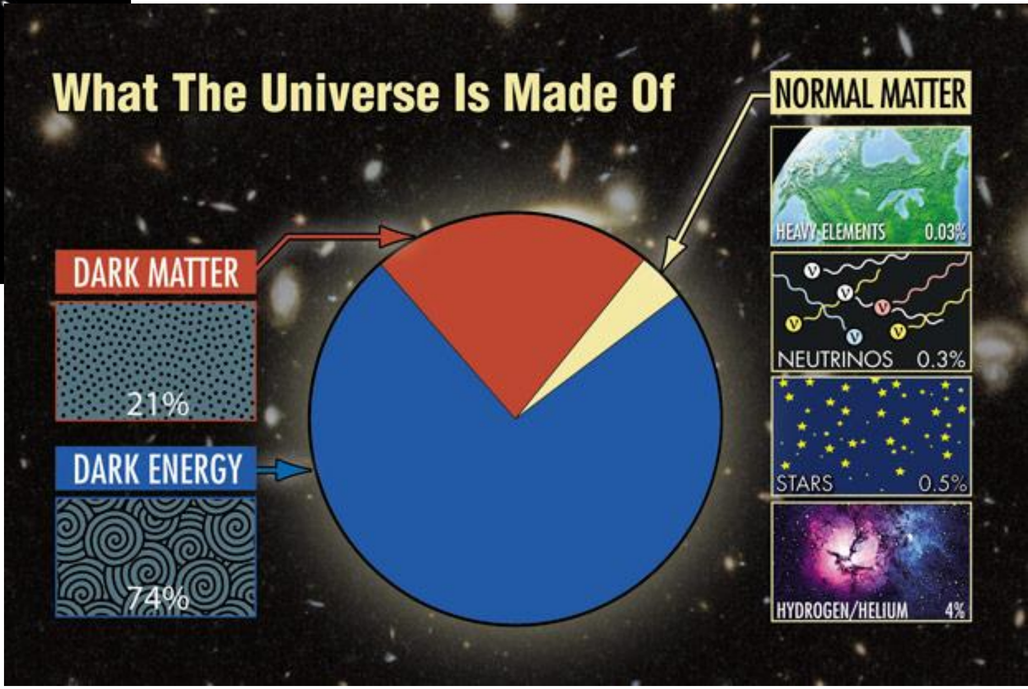
University of Chicago

DARK ENERGY SURVEY

Expansion and Composition of the Universe

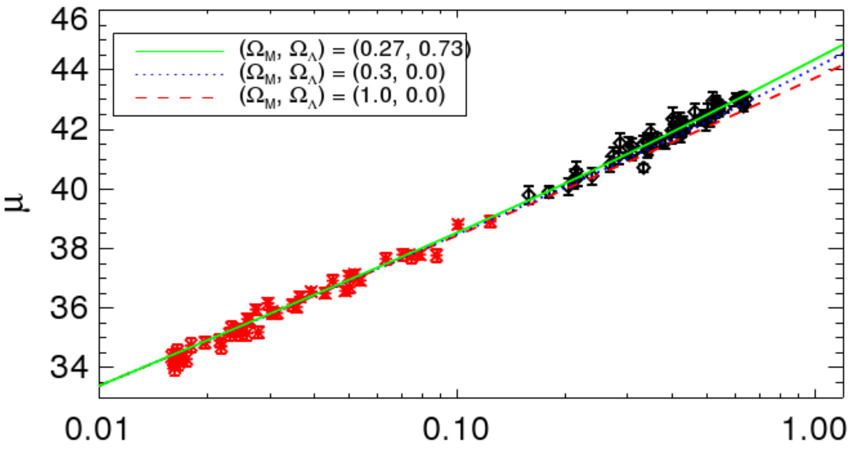


Courtesy: http://hetdex.org



Evidence from Acceleration from Type Ia SNe

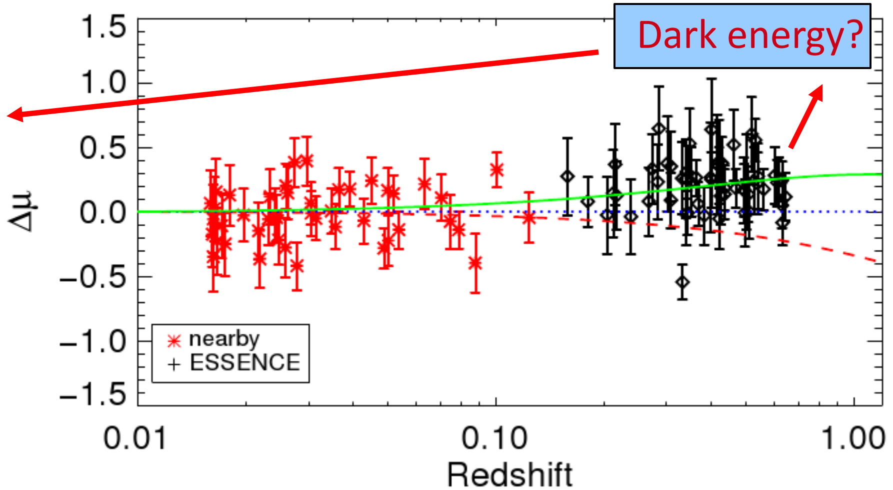
Credit: European Southern Observatory
Source: http://www.eso.org/public/videos/eso0943b



Credit: W. M. Wood-Vasey et al. 2008, ApJ, 666, 694

Dark energy?

Just one problem: "best" model explaining dark energy is off by a factor of 10^{120}



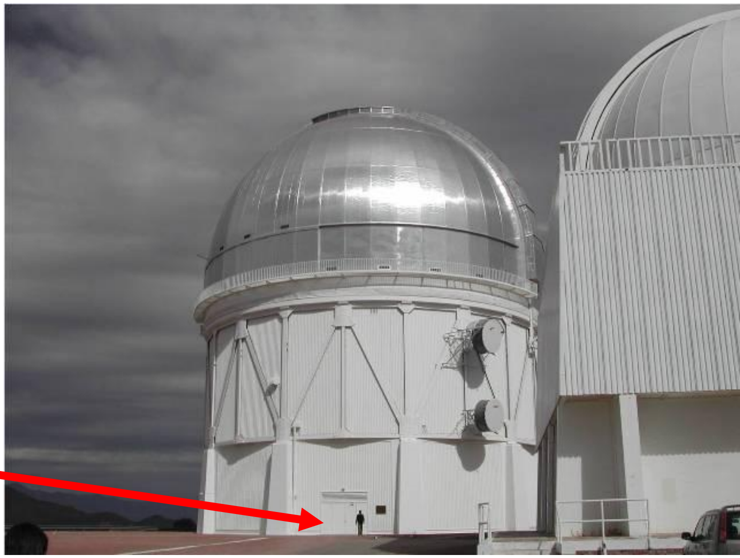
Dark Energy Survey (DES)

DES will survey 5000 square degree of sky and provide new 500Mpixel CCD camera (DECam) for Blanco 4m telescope at the Cerro Tololo Inter-American Observatory (CTIO), Chile, in exchange for 525 survey nights over 5 years starting in 2011.

DE investigation via 4 independent probes:
1) Galaxy angular clustering
2) Weak gravitational lensing
3) Baryon acoustic oscillations
4) SN Ia distances

DES is expected to observe ~10^8 galaxies & will obtain redshifts for the South Pole Telescope survey.

Joe



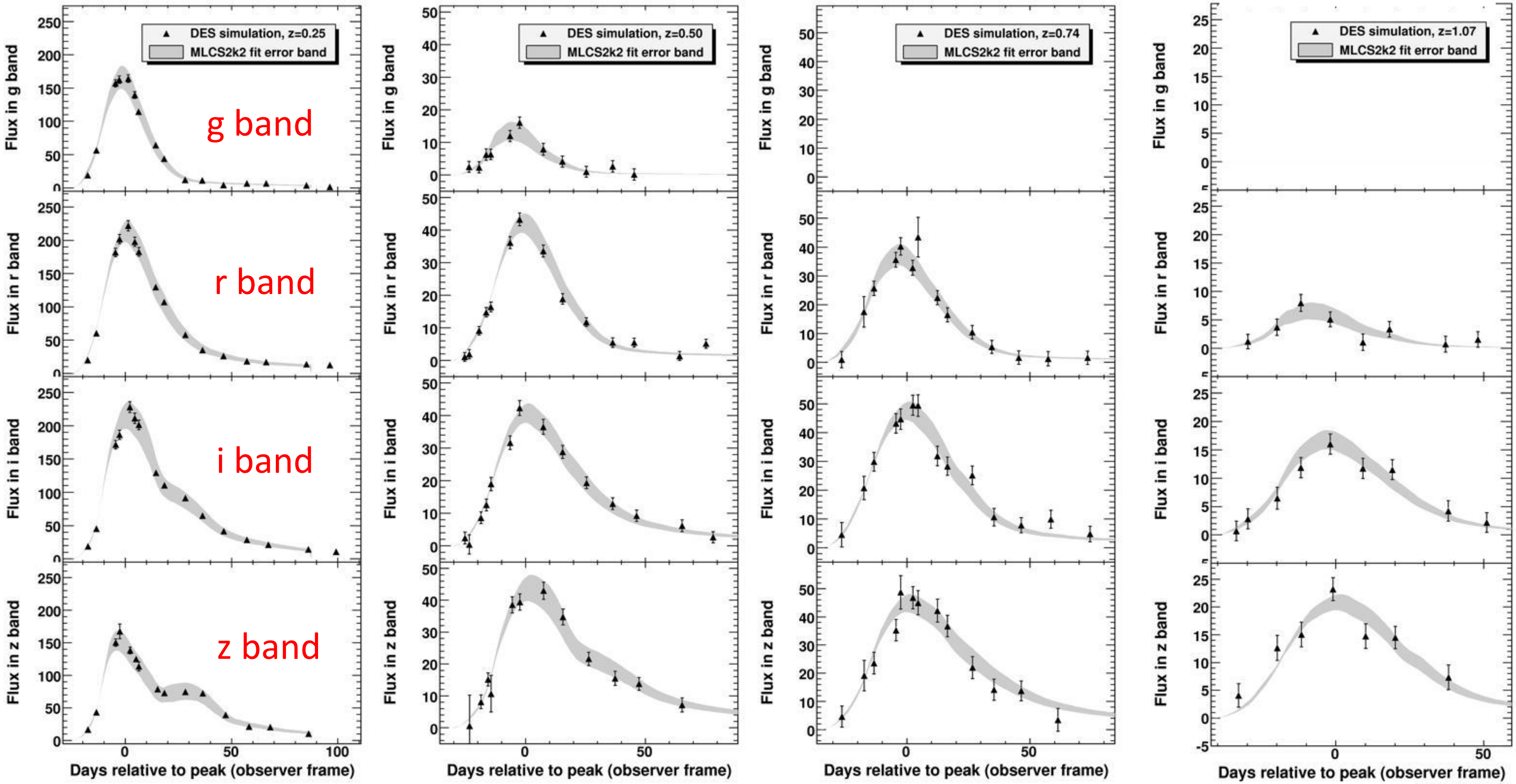
SNANA: SuperNova ANAlysis package for DES

R. Kessler (U. Chicago), J. P. Bernstein, S. Kuhlmann, & H. Spinka (ANL)

- Also used by SDSS & LSST
- Software suite for simulating and fitting SN light curves
- Motivation was a more accurate and complete study of DES-SN capabilities including DES CCD and filter characteristics, CTIO sky fluctuations using Essence data inputs, dust extinction effects, etc.
- Uses various models (e.g., MLCS2k2, SALT-II, stretch, etc.)
- Models and fits both Ia and non-Ia SNe
- Public URL: http://www.sdss.org/supernova/SNANA.html

Example DES Simulated SN Ia Light Curves

Redshift 0.25 Redshift 0.50 Redshift 0.74 Redshift 1.07



Selection cuts for DES supernovae
1. At least 5 total epochs above a very small, but non-zero, signal-to-noise threshold
2. At least one epoch before and at least one 10 days after the B-band peak
3. At least one filter measurement with a signal-to-noise above 10
4. At least two additional filter measurements with a signal-to-noise above 5

g band: 400 – 550 nm

r band: 560 – 710 nm

i band: 700 – 850 nm

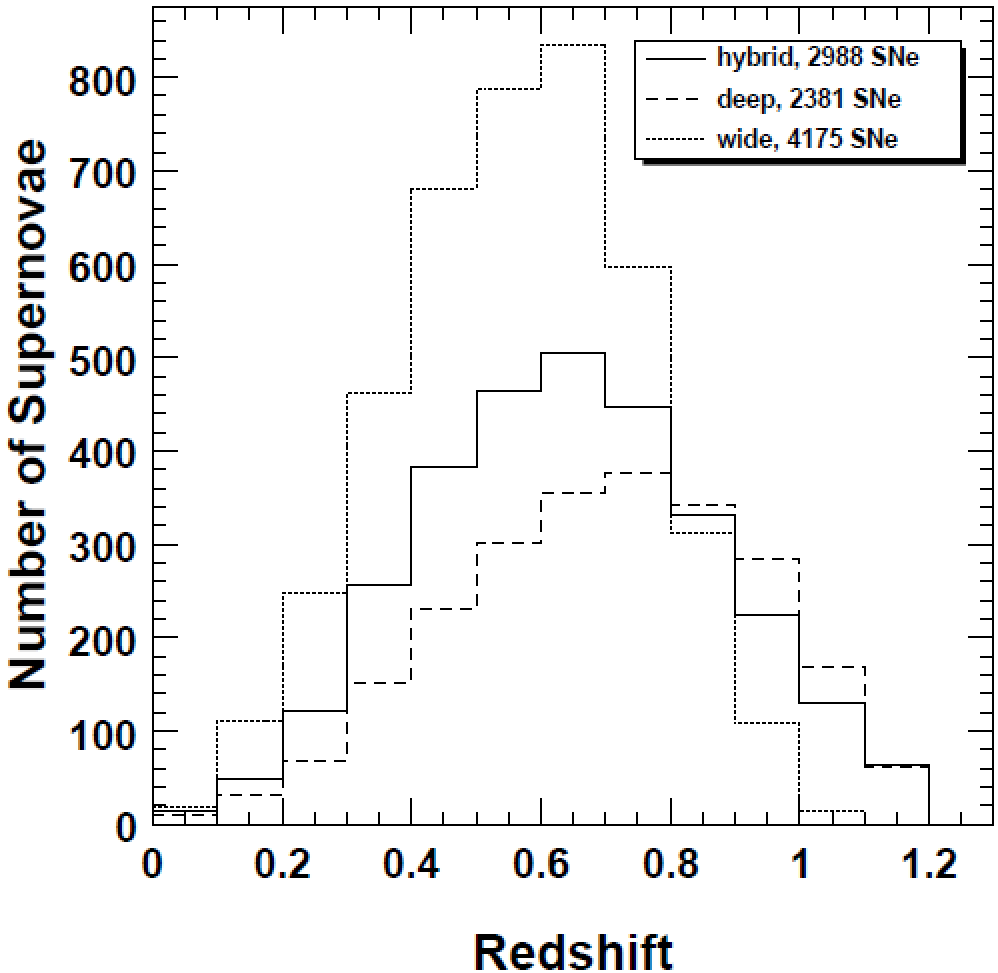
z band: 860 – 1000 nm

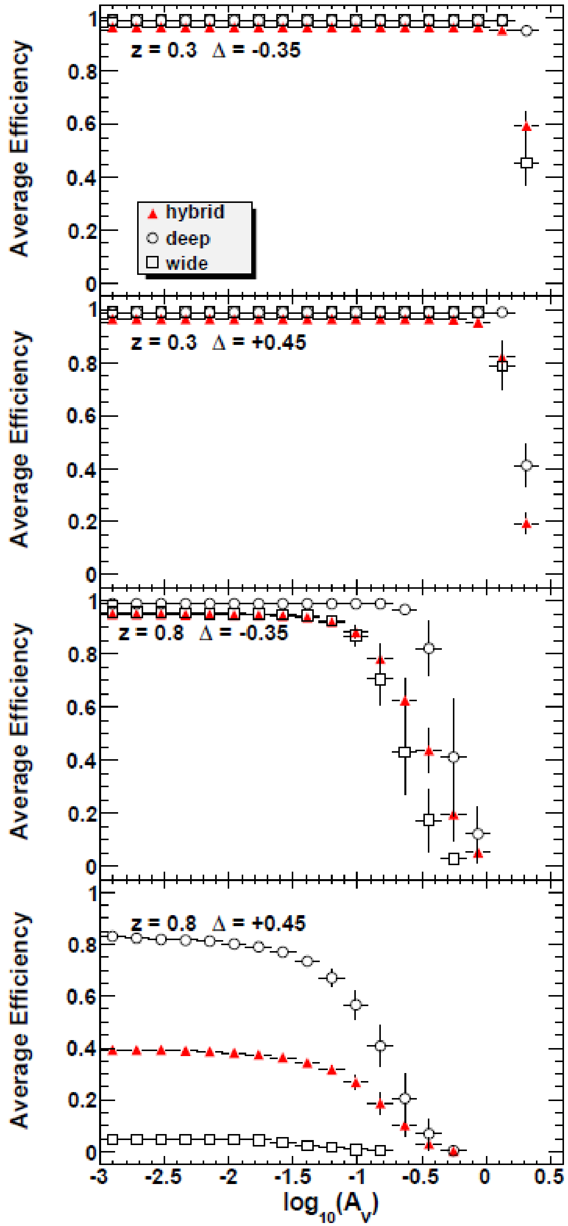
Filter	Range (nm)	Exposure time (s)
g	400–550	300
r	560–710	1200
i	700–850	1800
z	850–1000	4000
Z_1	850–970	n/a
Z_2	850–920	n/a
Y	970–1020	n/a

Deep; Wide = Deep/3

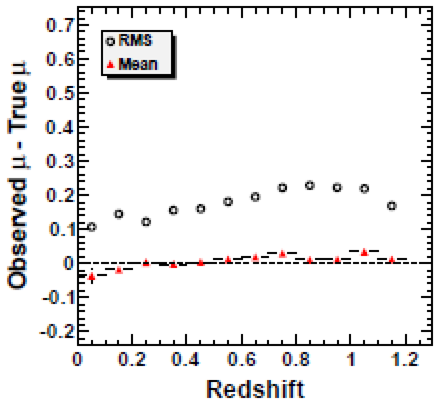
Number of SNe and Selection Efficiency

DARK ENERGY SURVEY

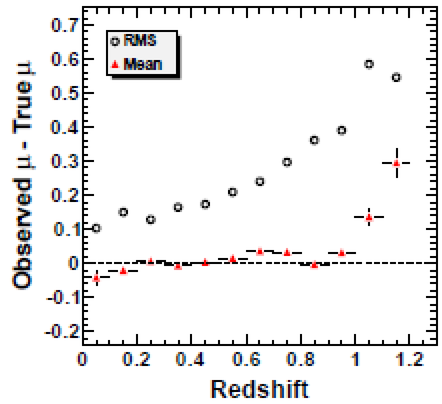




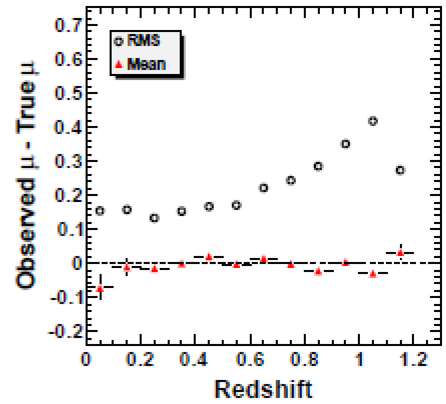
True Distance Recovery



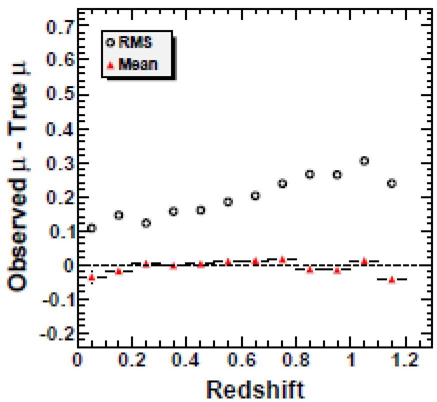
(a) MLCS2k2 fit for hybrid strategy with full priors.



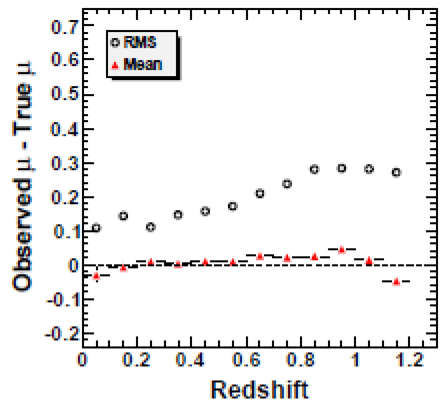
(b) MLCS2k2 fit for hybrid strategy with flat priors.



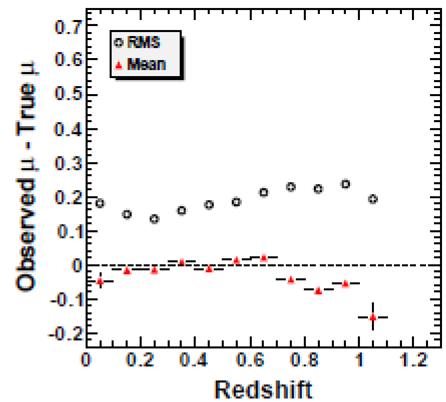
(c) SALT2 fit for hybrid strategy.



(d) MLCS2k2 fit for hybrid strategy with partial prior without efficiencies applied.



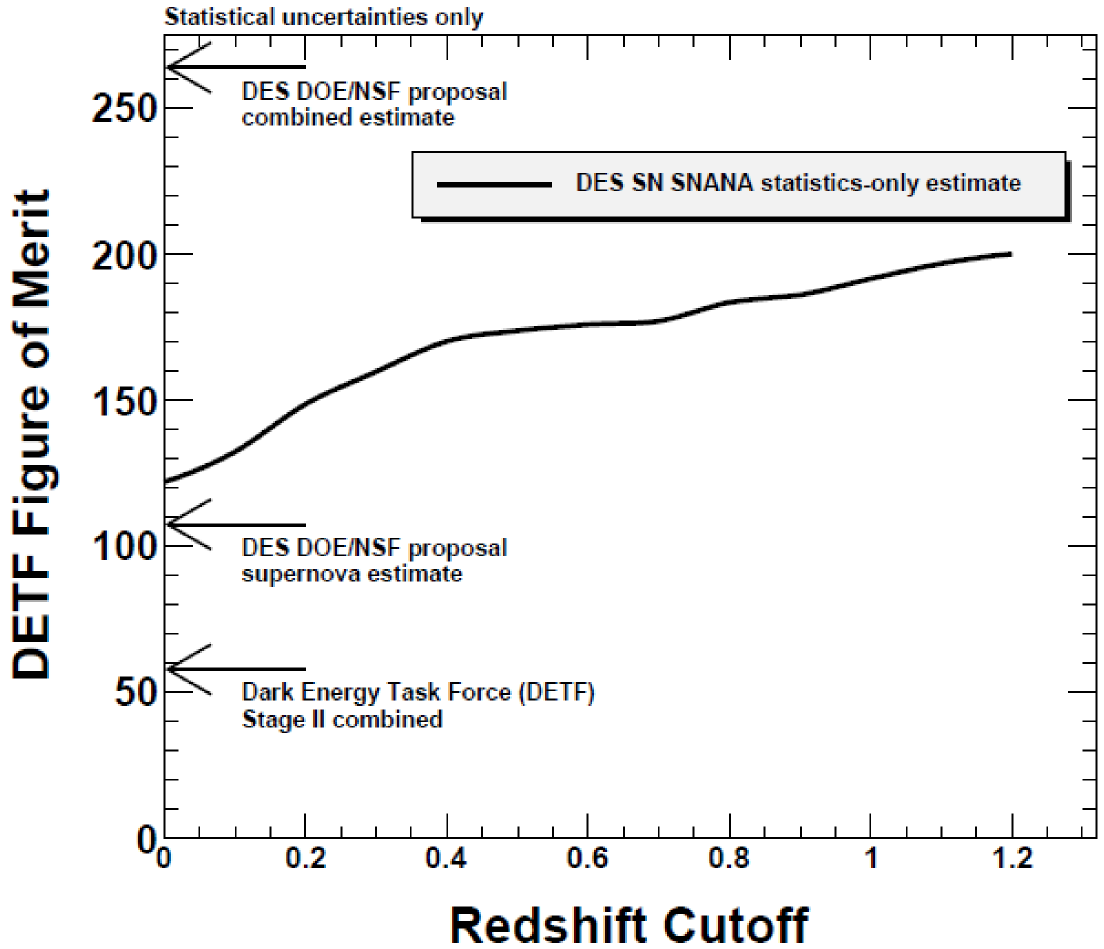
(e) MLCS2k2 fit for deep strategy with partial prior without efficiencies applied.



(f) MLCS2k2 fit for wide strategy with partial prior without efficiencies applied.

Spectroscopic Redshift Cutoff

- DES will rely on photometric SN identification and redshifts (z; initially)
  - photometric z – true z width ~ 4% using host galaxy colors only
  - when SN colors used with host as prior, improves to ~2.5%

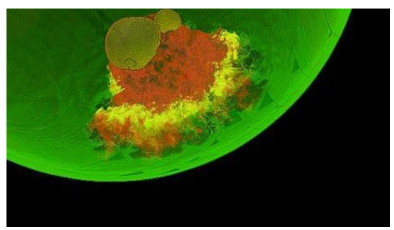
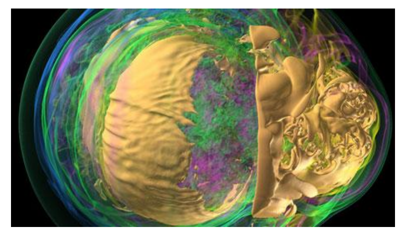
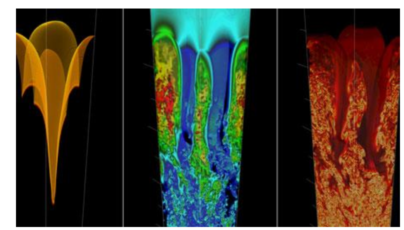
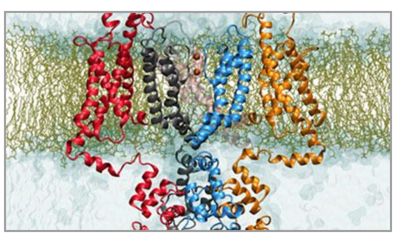
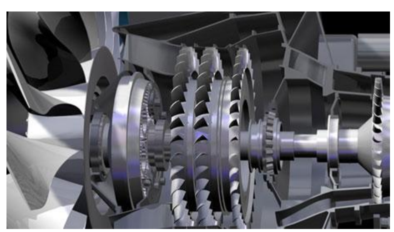
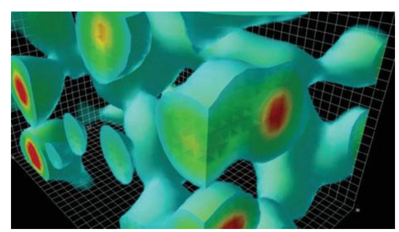
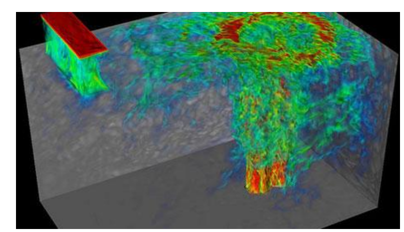


Additional Simulation Results

- Detailed contamination study indicates level significant but manageable
- 3-year overlap with the VIDEO IR survey
  - allows for combined optical+IR sample of few hundred SNe
  - VERY useful for unraveling systematic effects
  - optical+IR SNANA simulation capabilities in place
- Filter zeropoint shift study: 0.01 leads to 0.03 shift in DE EOS parameter
- Other systematics still under evaluation
  - mostly “community-wide”, e.g., dust, with many working to reduce
  - can improve zeropoint systematic with PreCam pre-DES calibration survey

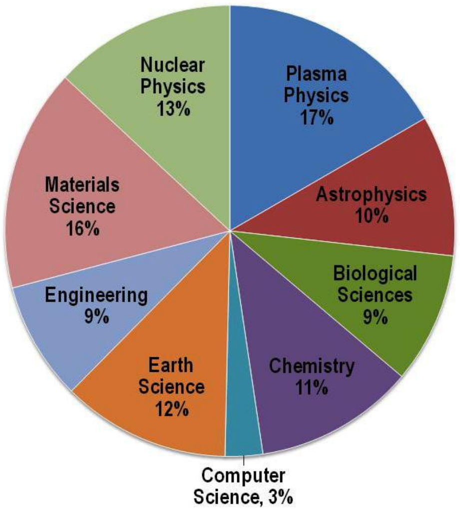
The Argonne Leadership Computing Facility (ALCF)

- Since 2006, the ALCF has provided the computational science community with a leading-edge computing capability dedicated to breakthrough science and engineering.
- One of two DOE national Leadership Computing Facilities
- Supports the primary mission of DOE’s Office of Science Advanced Scientific Computing Research (ASCR) program to discover, develop, and deploy the computational and networking tools that enable researchers in the scientific disciplines to analyze, model, simulate, and predict complex phenomena important to DOE.

INCITE 2010 Awards

- 35 new projects and 34 renewal projects
- 41% of new submittals and 83% of renewals received awards



U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

Innovative and Novel Computational Impact on Theory and Experiment

- Solicits large-scale, computationally intensive research projects
  - **to enable high-impact scientific advances**
- Open to all scientific & engineering researchers and organizations worldwide
  - **including universities, laboratories and companies**
- Provides large computer time and data storage allocations
  - **average award in 2010 was 23 million hours**

http://hpc.science.doe.gov/

Discretionary Allocations

Discretionary allocations are "start up” awards made to potential future INCITE projects. Projects must demonstrate a need for leadership-class resources. Proposals must include a description of the science problem to be addressed.

Availability	Year round to industry, academia, laboratories and others.
Duration	Three to six months, renewable.
Award Size	Varies based on the application and its readiness/ability to scale; generally from the low tens of thousands to the low millions.
Available Systems	Intrepid – Used for production scientific and engineering computing. Surveyor – Used for tool and application porting, software testing and optimization, and systems software development.

https://wiki.alcf.anl.gov/index.php/Discretionary_Allocations

Blue Gene/P Overview

Intrepid System
40 Racks

1 PF/s
144 TB

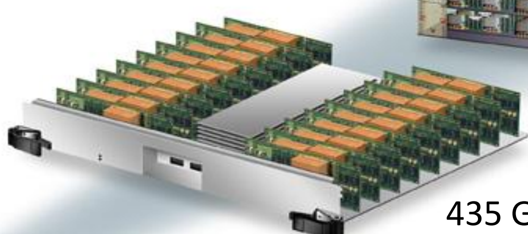
Rack

Cabled 8x8x16

32 Node Cards
1024 chips, 4096 procs

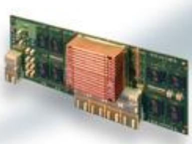
14 TF/s
2 TB

Node Card
(32 chips 4x4x2)
32 compute, 0-2 IO cards



435 GF/s
64 GB

Compute Card
1 chip, 20 DRAMs



13.6 GF/s
2.0 GB DDR
Supports 4-way SMP

Chip
4 processors

850 MHz
8 MB EDRAM

Maximum System
256 racks
3.5 PF/s
512 TB

Front End Node / Service Node
System p Servers
Linux SLES10

HPC SW:
Compilers
GPFS
ESSL
Cobalt

On the Road to Exascale

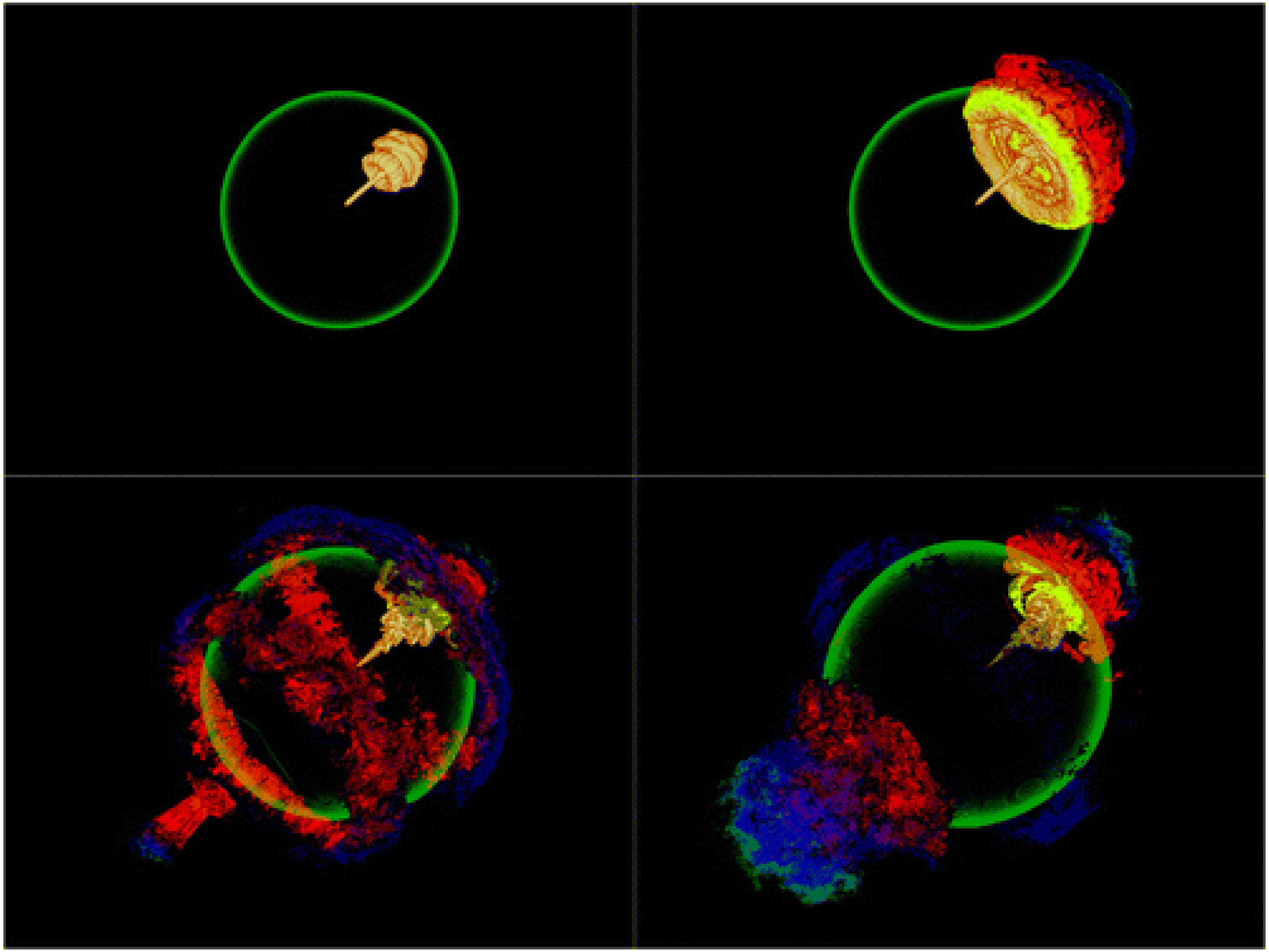
In early 2012, the Argonne Leadership Computing Facility will install *Mira*, a next-generation Blue Gene system.

- 10 petaflops system
- 0.75 million cores
- 16 cores per node
- 1 GB of memory per core

Pursuing Fundamental Physics with Intrepid

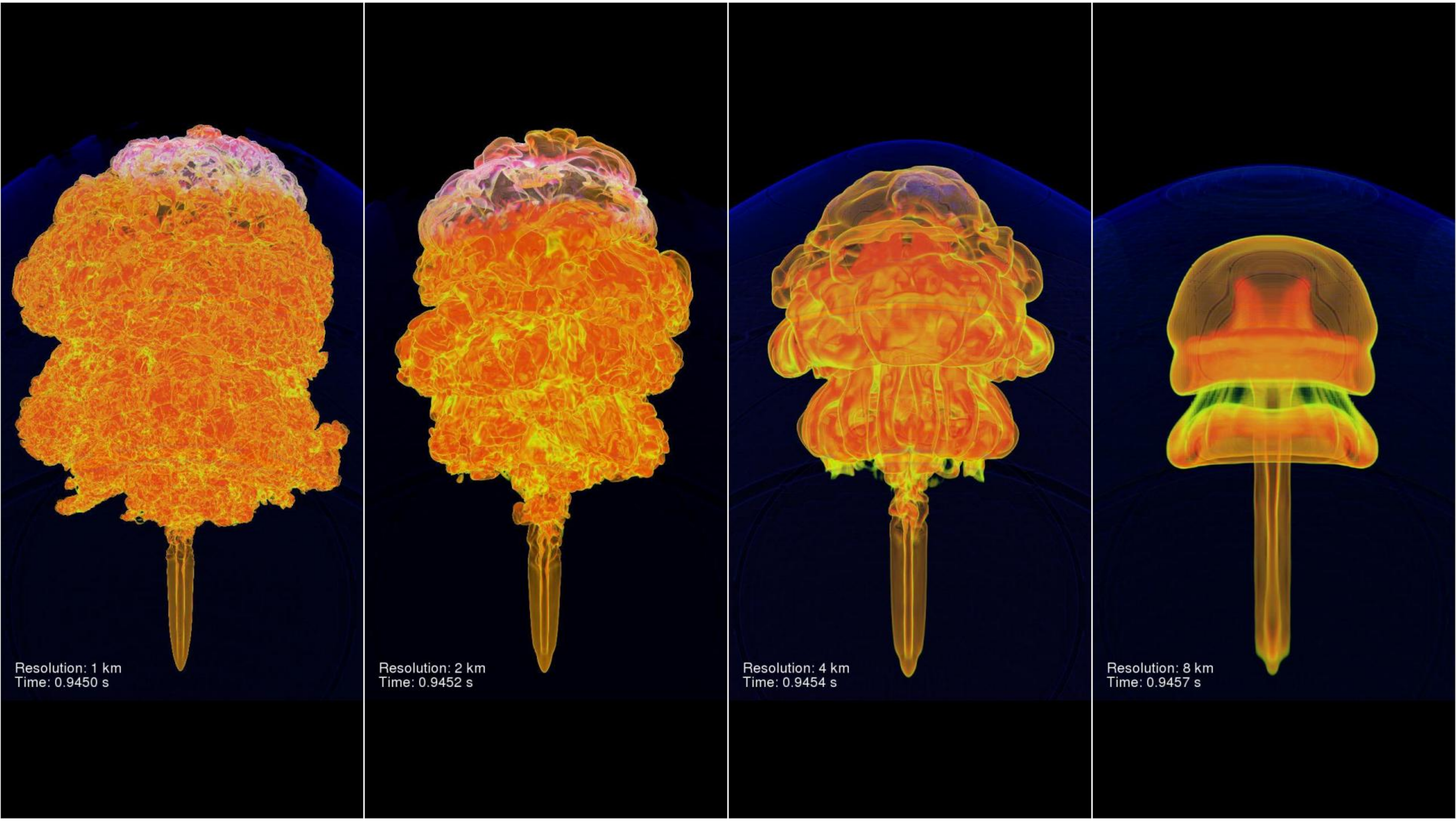
- SN Ia explosion modeling
  - Argonne – FLASH Center – Others collaboration
  - simulate white dwarf detonation and explosion using FLASH code
  - seeking to understand SN Ia brightness from fundamental physics
- SN Ia radiative transfer
  - PHOENIX
    - Initial discussions with U. Chicago people have occurred
    - Argonne FY 2011 LDRD for non-LTE library development pending
    - Initial BG/P scaling by Daan van Rossum shows promise
  - SEDONA
    - Dan Kasen's code (Kasen, Thomas, Nugent 2006, ApJ, 651, 366 (2006)
    - 2D test runs successfully performed on BG/P
    - Near ideal scaling for a minimally parallel case
- Computational cosmology
  - simulate large scale structure of Universe with FLASH
  - pursuing BG/P optimization & scaling studies w\ Paul Ricker & Boyana Norris

3-D SN Ia Simulations



Jordan et al. 2008, ApJ, 681, 1448

Buoyancy-driven Turbulent Nuclear Combustion



Credit: Brad Gallagher

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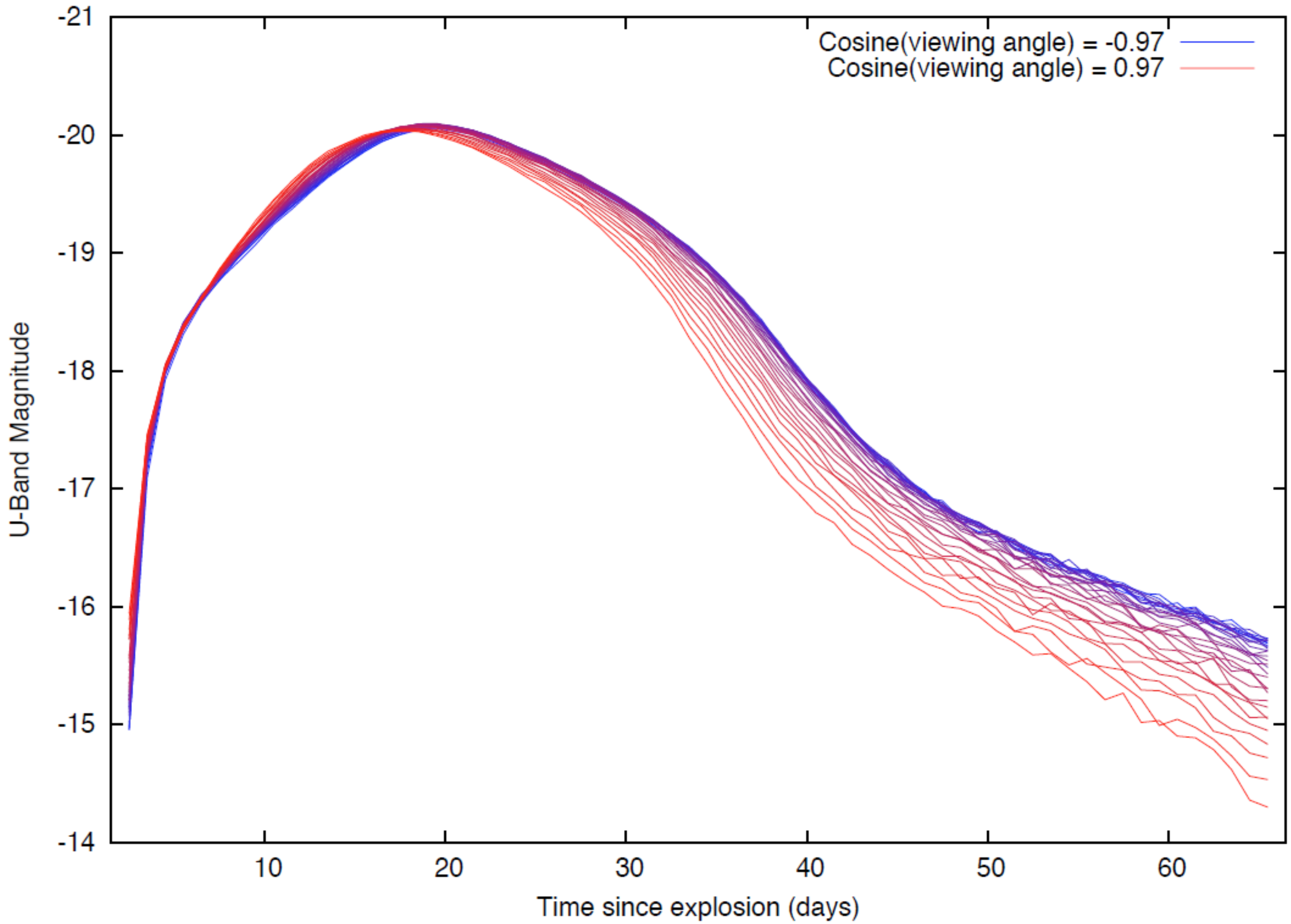
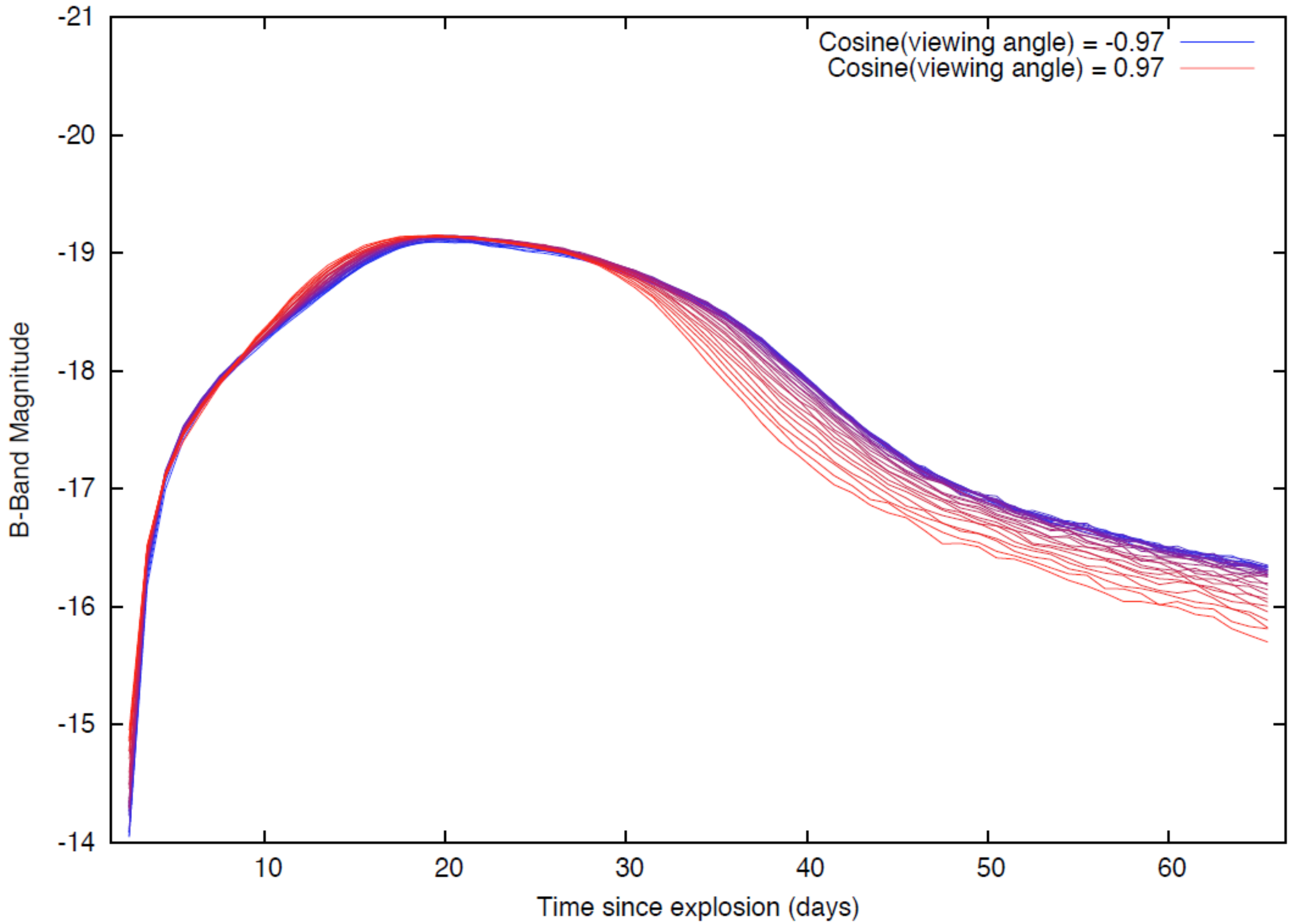
Ultraviolet Brightness vs. Time



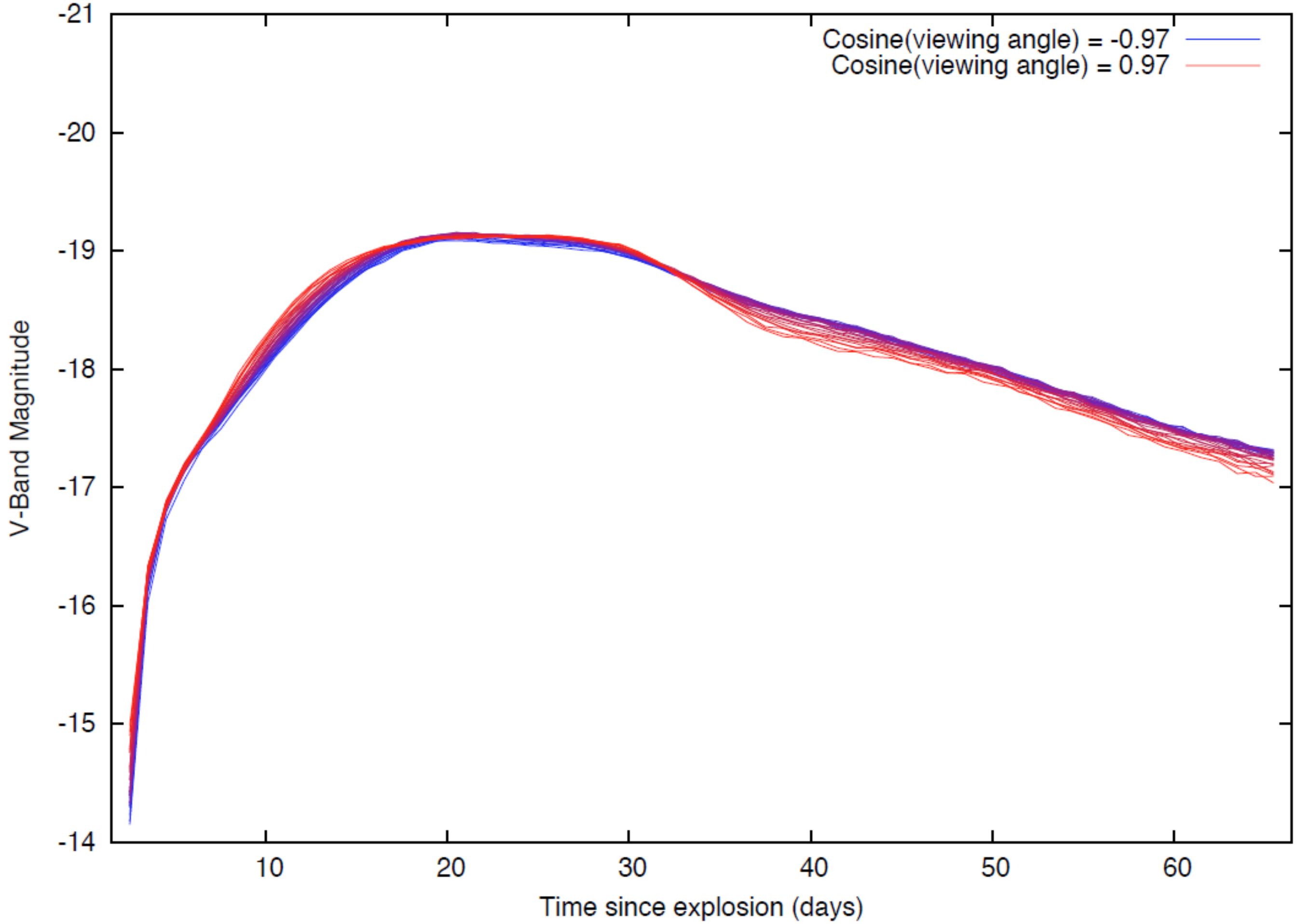
Credit: Benedikt Diemer

Blue Brightness vs. Time



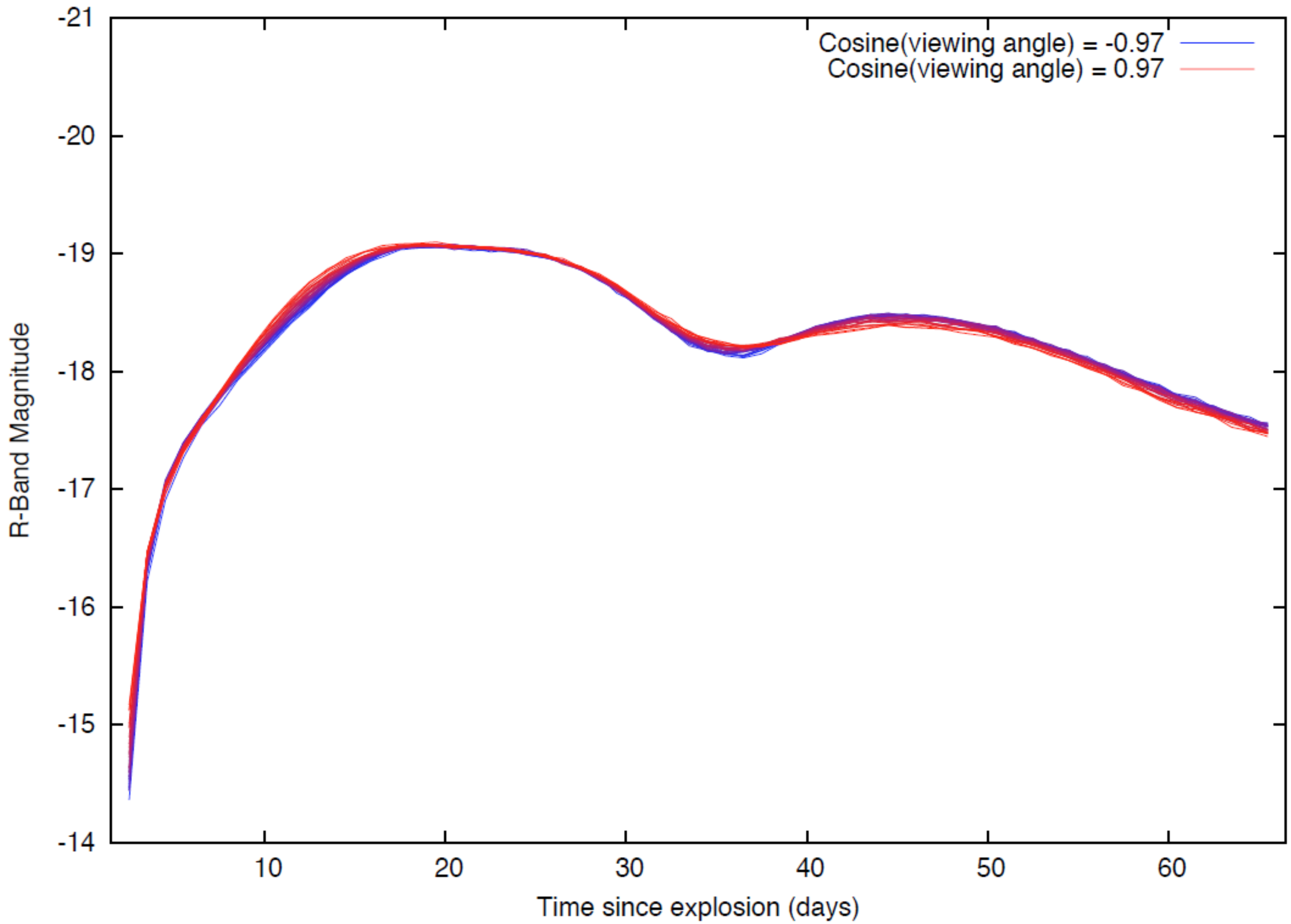
Credit: Benedikt Diemer

Green Brightness vs. Time



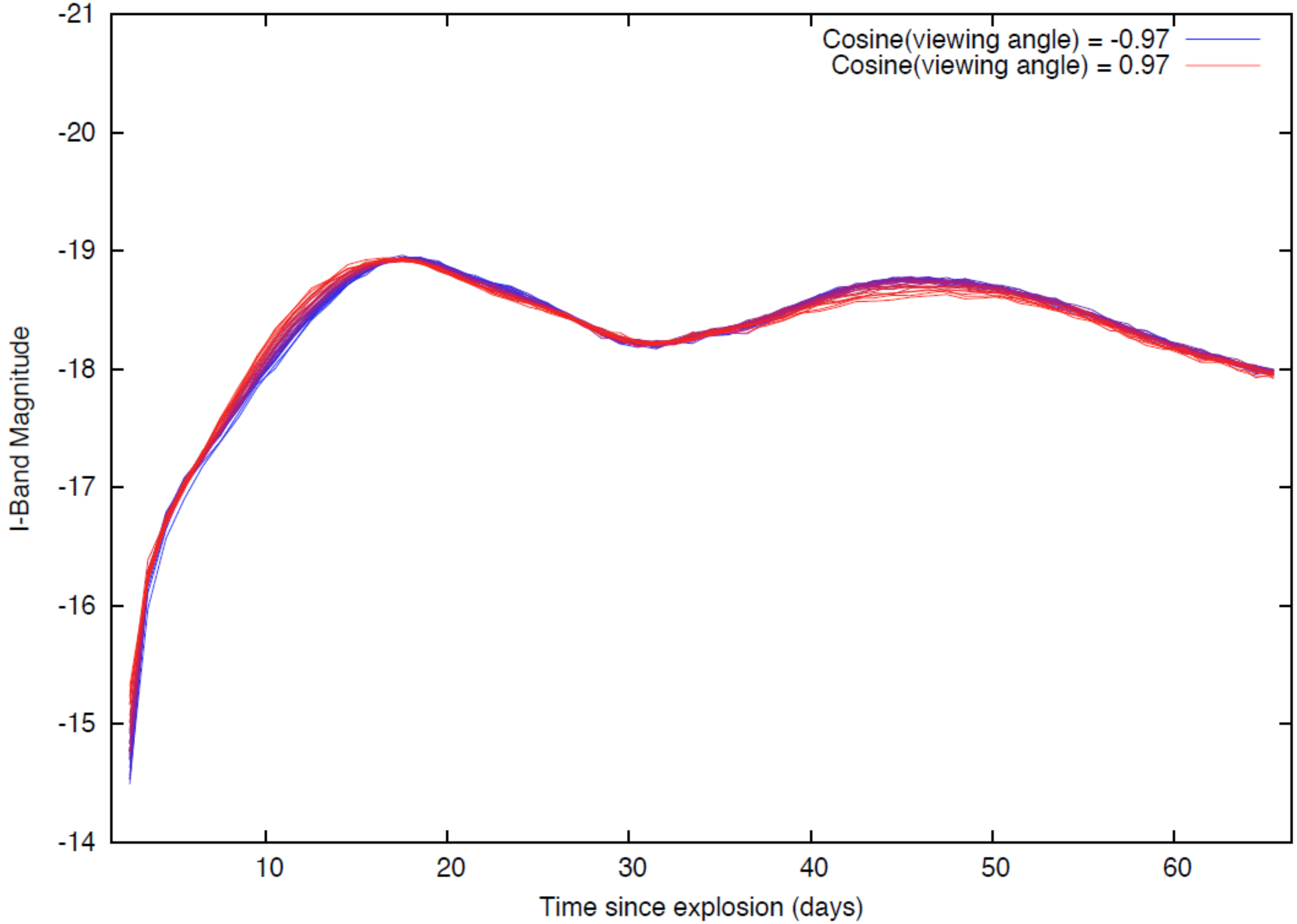
Credit: Benedikt Diemer

Red Brightness vs. Time



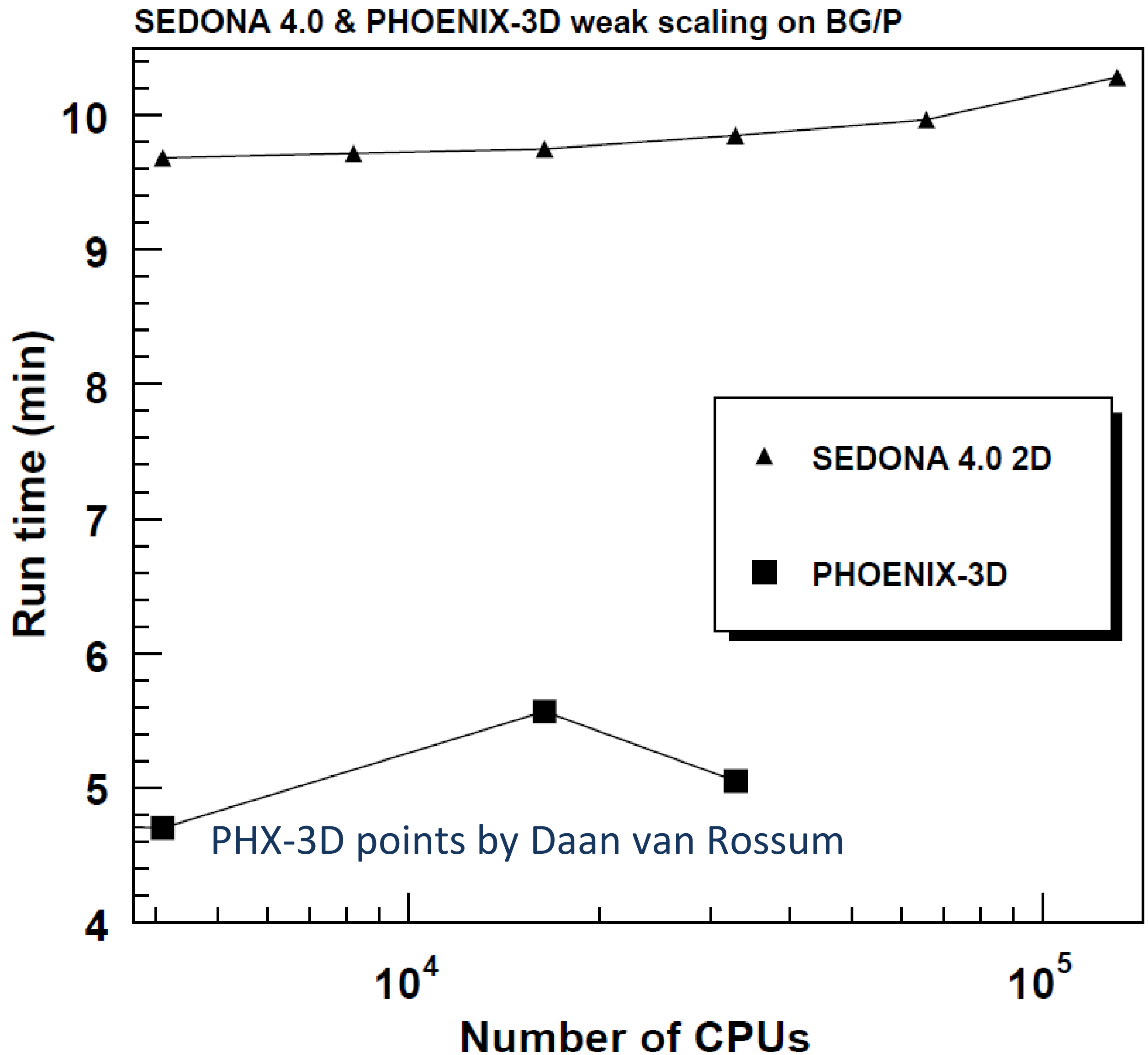
Credit: Benedikt Diemer

Infrared Brightness vs. Time



Credit: Benedikt Diemer

Weak Scaling On BG/P (SEDONA: full replication)



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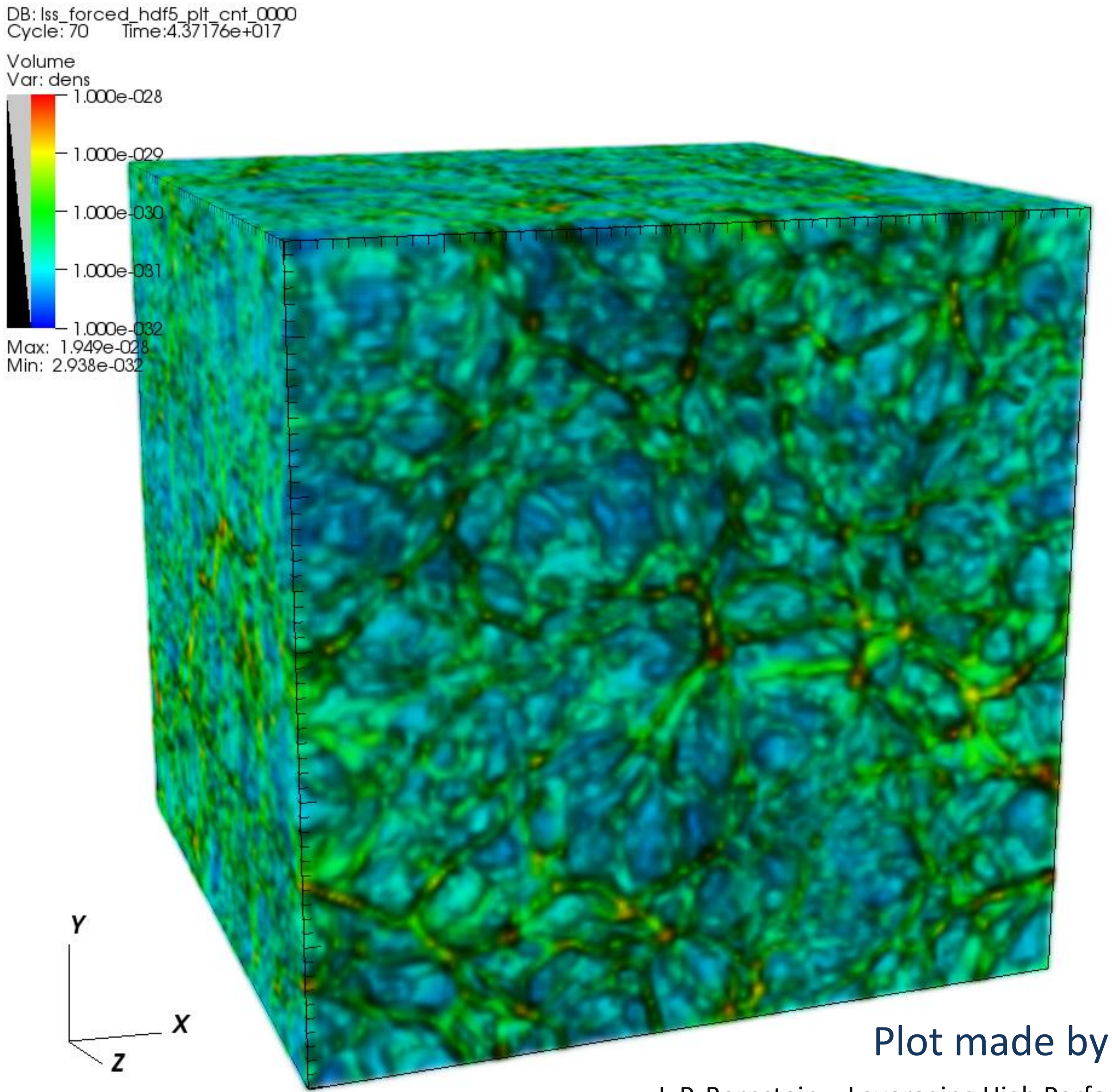
BG/P Test: 512^3 particles w/ hydro (6 refinement levels)



Plot made by Steve Kuhlmann

Active Work

- Radiative transfer : relaxing Local Thermo. Equilibrium (LTE) assumption
  - no existing codes can handle non-LTE assumption at HPC scale
  - Argonne FY 2011 LDRD for non-LTE library development pending (JPB PI)
- Computational cosmology
  - MUCH larger simulations needed
  - working on 1024^3-particle proof of principle problem
  - ultimate technical goal is 4096^3 particles and more
  - science: study voids in Universe – requires extreme force resolution
  - Boyana Norris working on optimization and OpenMP studies

Summary & Conclusion

- March to precision cosmology demands HPC simulations
- Future survey interpretation, e.g., DES, Pan-Starrs, LSST, require sims
- ANL actively engaged on two fronts
  - supernova explosion modeling
  - computational cosmology
- Many applications suitable to petascale and beyond
- ANL improving leadership capability w/ senior computational hires